Isopropyl carbamate

1746-77-6 | DTXSID9051795

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.27e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.59e-01

Confidence level: 5.42e-01

Nearest Neighbors from the Training Set

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Urethane
Measured: 2.62e-01
Predicted: 3.29e-01

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Tetraethyl orthosilicate
Measured: 7.00e-01
Predicted: 2.76

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1,1,1-Trichloro-2,2,2-trifluoroethane
Measured: 1.00e-03
Predicted: 702

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Ethyl chloroacetate
Measured: 9.05e-01
Predicted: 7.43